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Quality Assurance and Quality Control Plan for the 1985 NAPAP (National Acid Precipitation Assessment Program) Emissions Inventory (November 1988)

Alliance Technologies Corp., Chapel Hill, NC

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QUALITY ASSURANCE AND QUALITY CONTROL PLAN FOR THE 1985 NAPAP EMISSIONS INVENTORY

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16. ABSTRACT The paper identifies the quality assurance and quality control (QA/QC) objectives that must be met to create a comprehensive and accurate emissions inventory and summarizes the QA/QC plan specifically designed for the 1985 inventory to meet these objectives. The data quality objectives, priorities, and constraints for the collection of the 1985 inventory data are reviewed. QA/QC checks of both state data and the completed inventory are discussed. Guidelines for data processing, documentation, and the calculation of data quality indicators are reviewed. A fundamental objective of the National Acid Precipitation Assessment Program (NAPAP) research program is the location and quantification of natural and anthropogenic emissions that may contribute to acid deposition. To achieve this objective, NAPAP's Task Group and Emissions and Controls is conducting a multi-year research effort to develop an accurate and comprehensive inventory of 1985 emissions from sources thought to be important in acid deposition processes. Most of the 1985 emissions data for this inventory are being collected and analyzed by state air pollution control agencies and the U.S. EPA.

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ABSTRACT

The National Acid Precipitation Assessment Program (NAPAP) was established by Congress in 1980 to coordinate and expand research on problems posed by acid deposition in and around the U.S. One fundamental objective of NAPAP's research program is the location and quantification of natural and anthropogenic emissions that may contribute to acid deposition. To achieve this objective, NAPAP's Task Group on Emissions and Controls is conducting a multi-year research effort to develop an accurate and comprehensive inventory of 1985 emissions from sources thought to be important in acid deposition processes. Most of the 1985 emissions data for this inventory are being collected and analyzed by State air pollution control agencies and the U.S. Environmental Protection Agency. This paper identifies the quality assurance and quality control (QA/QC) objectives that must be met to create a comprehensive and accurate inventory and summarizes the QA/QC plan specifically designed for the 1985 inventory to meet these objectives. The data quality objectives, priorities, and constraints for the collection of the 1985 inventory data are reviewed. QA/QC checks of both State data and the completed inventory are discussed. Guidelines for data processing, documentation, and the calculation of data quality indicators are reviewed.

INTRODUCTION

The "Acid Precipitation Act of 1980" (Title VII of P.L. 96-294) established a long term program to coordinate and expand research on problems posed by acid deposition in and around the U.S. Among the priority research objectives that Congress identified for this National Acid Precipitation Assessment Program (NAPAP) was the development of an accurate and comprehensive emissions inventory of natural and anthropogenic sources that may contribute to the formation of acid precipitation. Currently, NAPAP's Task Group on Emissions and Controls is working with the U.S. Environmental Protection Agency (EPA), State air pollution control agencies, and Environment Canada to develop an emissions inventory for calendar year 1985 that will meet this objective. The U.S. EPA effort is managed by the Office of Research and Development (ORD), Air and Energy Engineering Research Laboratory (AEERL).

This paper discusses the quality control procedures that have been developed for this inventory to ensure that its emissions data represent the most accurate estimates of 1985 emissions possible. At the outset of this discussion, it must be acknowledged that the nature of emissions inventories precludes the application of conventional quality assurance and quality control (QA/QC) procedures to the acquisition of inventory data. Traditionally, these procedures are developed to govern the acquisition and analysis of environmental measurements that will be used for research or decision making. However, emissions inventories are rarely based on environmental measurements. Rather, they are developed from estimates of emissions which are derived from emissions factors and activity indicators. In this context, the fundamental concepts of data accuracy and QA (assessing the difference between measured and true values) do not apply. Thus, procedures for verifying the reasonableness--as opposed to the accuracy--of emissions inventories are limited to QC checks.

The development of these procedures is complicated further by the size of the 1985 inventory and its component data bases. For example, the anthropogenic point source data base maintained by EPA's National Emissions Data System (NEDS) contains 50 data elements for each of about 250,000 emission points--or about 66 million bytes of data. The final 1985 emissions inventory, which will include these point source data, will contain hourly emissions estimates for 29 pollutant species along with 100 area source emissions categories for each of 63,000 grid cells (each cell is a geographic area roughly 20 km square)--or about 4 billion bytes of data. For data bases of this magnitude, QA/QC procedures must be maintained and applied on large computers.

The following discussion of QA/QC procedures for the 1985 NAPAP Emissions Inventory will focus on two areas: procedures developed to check the reasonableness of emissions data for point or stationary sources of emissions; and procedures developed to analyze the reasonableness of emissions estimates in the final inventory.

QUALITY CONTROL FOR POINT SOURCES

The QA/QC procedures focus on the largest point source emission categories: electric utilities, petroleum refining, cement manufacturing, pulp and paper mills, motor vehicle coating, and iron and steel mills. In addition, QA/QC procedures focus on several data elements that have been identified as priorities for NAPAP research; i.e. emissions estimates, unit process identifiers (source classification codes), control equipment and efficiencies, fuel and operating rate data, location, throughput, and temporal profile data. All five criteria pollutants--nitrogen oxides (NO_x), sulfur oxides (SO_x), volatile organic compounds (VOC), total suspended particulates (TSP), and carbon monoxide (CO)--are believed to play a role as acid rain precursors and are included in the NAPAP inventory. The point source QA/QC methodology focuses on NO_x, SO_x, and VOC because they are expected to play major roles.

A major objective of the point source data base QA/QC checks is to effectively communicate their results to field inventory personnel who are most knowledgeable about sources in their States. For this reason, the point source QA/QC process for 1985 is a three-step screening process. The first step, at the field level, involves State and EPA regional office personnel. The second step, which occurs after the data are submitted to NEDS, is a search for systematic errors and omissions in the data. The third step is the return of detailed QA/QC documents outlining any problems found with the data to the States so that they may comment on and correct the data. A flow chart of the QA/QC procedures is shown in Figure 1.

First Level Field Screening

For the 1985 inventory, standard NEDS programs (e.g., NE061) have been redesigned for NAPAP to focus on high priority data elements. The EPA Regional Offices and States have been provided with the NE061 QA/QC computer programs, which generate two standard edit checking reports. The first of these is the NE061 rejection report, which lists any computer cards that were rejected, briefly describes the error, and highlights the erroneous data items. Cards that are rejected may have invalid State, county, Air Quality Control Region (AQCR), plant, or point identifiers (IDs). The Source Classification Code (SCC), action code, transaction type, or card number may be invalid. When data are rejected in this fashion, States correct the errors, and resubmit the information. The second standard NE061 edit checking report is the warning report. Warnings are generated if certain data items are missing, exceed limits established in the external data files, or are internally inconsistent. Example warning messages in these areas are:

Warning - annual operating rate is blank;
Warning - sulfur content not in range; and
Warning - stack diameter > 0.2 x stack height.

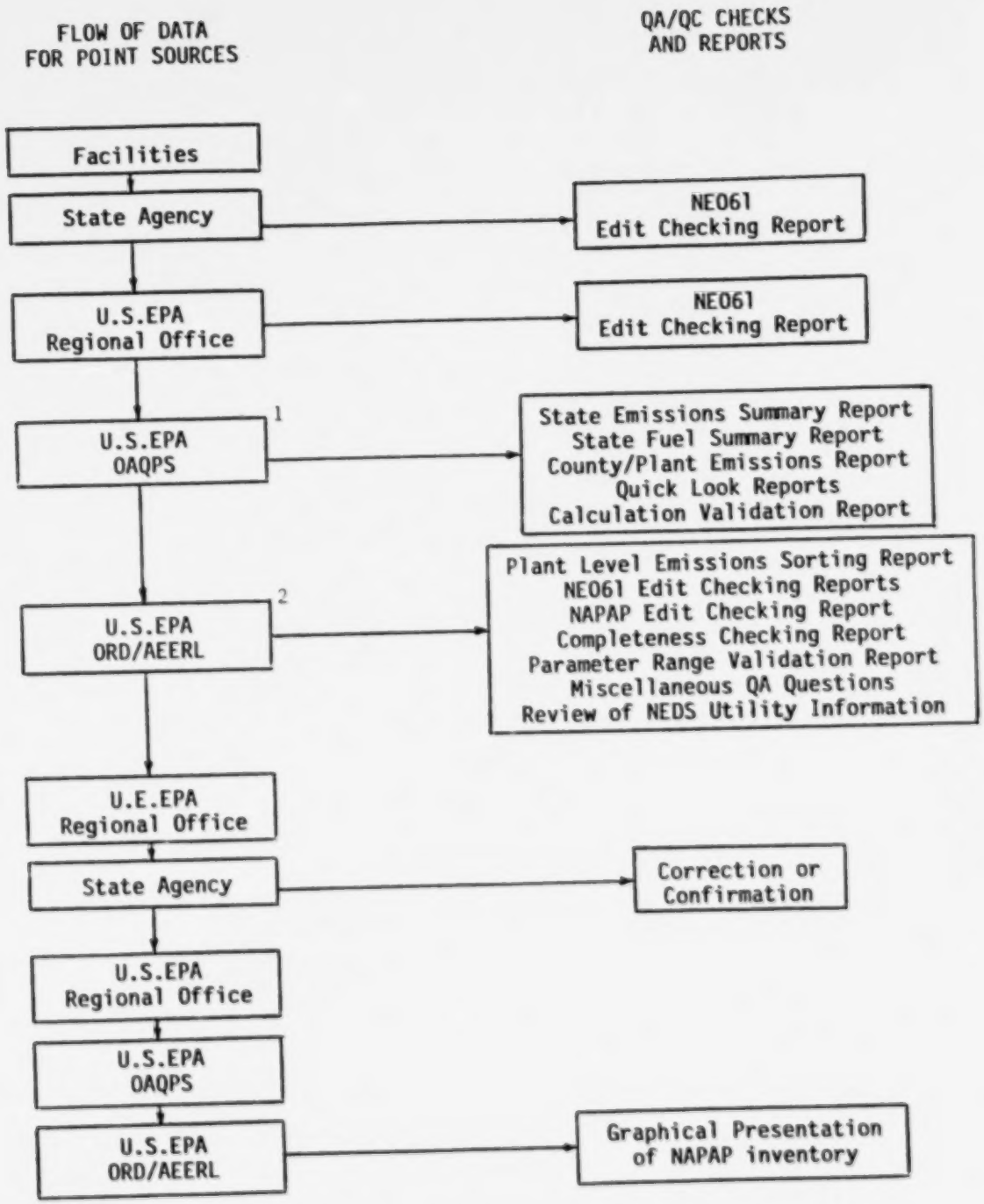

Figure 1. Flow Chart of Data Quality Control Procedures.

1 Office of Air Quality Planning and Standards
2 Office of Research and Development/Air and Energy Engineering Research Laboratory

Warning messages do not always indicate an error; however, EPA Regional Offices and States have been asked to verify that inventory data "flagged" by warning messages for facilities emitting greater than 1000 short tons (907 metric tons) per year (TPY) of NO_x, SO_x, or VOC are correct.

Second Level Data Screening

After State air pollution control agencies and EPA Regional Offices screen the 1985 NEDS data, they are submitted to the National Air Data Branch (NADB) at the U.S. EPA's Office of Air Quality Planning and Standards (OAQPS). At this point a second set of screening procedures (developed for the 1985 inventory) are applied. In this screening process, computerized programs are run to develop five standard reports, which indicate systematic errors:

State Emissions Summary Report;
State Fuel Summary Report;
County/Plant Emissions Report;
Quick Look Reports; and
Calculation Validation Report.

The State Emissions Summary Report is used for large scale comparisons of emissions data. It summarizes emissions data by combustion source type and, fuel type, and presents total statewide emissions for NO_x, SO_x, and VOC. These totals are compared to the previous year's totals and to previous emissions trends to ensure that there are no illogical changes.

The State Fuel Summary Report is used for large scale comparison of fuel consumption data. It is compared to the 1984 State Fuel Summary Report for each combustion category and for each type of fuel. Fuel consumed by electric utilities is also compared to the Department of Energy (DOE) Generating Unit Reference File (GURF).[1] State consumptions of coal, oil, and gas are compared to fuel delivery data provided by DOE.[2,3,4] Generally, coal consumption by point sources should equal coal delivered. Oil and gas consumption by point sources should be less than the fuel deliveries because area and mobile sources consume a large part of these fuels. The most frequent problem encountered during this analysis is over-reported consumption of fuels in the new NEDS submittals.

The County/Plant Emissions Report gives emissions by individual plants sorted by county. Other data fields, including year of record and location data, are also listed. This report is quickly scanned to ensure that the new data have a 1985 year of record.

NEDS can calculate emissions by multiplying the annual operating rate by an emission factor from the emission factor file. These emission estimates are computer calculated and are not as valid as estimated emissions data entered by the State agency. The Quick Look Reports are used to identify two possible problems. First, a check is made for instances where NEDS could have calculated positive emissions for a source that reported zero emissions. Small sources are ignored, but those with potential emissions exceeding 25 TPY

of NO_x, SO_x, or VOC are noted. Second, instances where the State requested that NEDS calculate emissions, but no emission factor exists in the emission factor file, are noted.

The Calculation Validation Report identifies any instance where NEDS could not allocate emissions from the point level to the SCC level. This generally occurs when one of the SCCs assigned to the point has no emission factor or if operating data are missing. If a decrease in emissions is found during the scan of the State Emissions Summary Report, then additional information on the possible miscalculation of emissions is found by reviewing the Calculation Validation Report, which prints out all instances where "Estimated point emissions differ from computed emissions by more than a factor of 3."

Return Of Quality Control Documents to the States

After the computer reports described above are produced, they are reviewed to determine whether or not the data are ready for a more extensive QA/QC procedure. If the data are deemed acceptable, the first QA/QC document for the States data is prepared. After the QA/QC document is prepared it is sent to the State and EPA Regional Offices for corrective action or confirmation of suspect data. The first QA/QC document has six sections:

Plant Level Emissions Sorting Report,
NE061 Edit Checking Reports,
NAPAP Edit Checking Report,
Completeness Checking Report,
Parameter Range Validation Report, and
Miscellaneous QA/QC Questions.

These include both computerized and manual checks and focus on the NAPAP high priority data items.

The Plant Level Emissions Sorting Report lists all of the facilities sorted by NO_x, SO_x, and VOC. Confirmation of any emission estimates received to date is indicated on this report. This report enables the State to view its sources ranked by emissions. It also highlights problems with the confirmation status, and shows which facilities have points with emissions status calculated by NEDS. This report is augmented with a breakdown by facility of points that have NEDS-calculated emissions.

The NE061 Report contains the results of the NE061 edit checking program (discussed above) for facilities with estimated emissions that exceed 1000 TPY of NO_x, SO_x, or VOC. The warnings generated are reviewed manually and categorized to ensure their validity. An example of warnings that need not be addressed is that on data for sources of CO emissions (a NAPAP non-priority pollutant).

The third section contains output from the NAPAP edit checking program. This group of computerized checks was established to augment the NE061 checks and searches for missing or internally inconsistent data. The checks focus on the NAPAP high priority data items, including stack parameters, operating data, and estimated emissions. A report is generated only for facilities with estimated emissions that exceed 1000 TPY of NO_x, SO_x, or VOC.

The Completeness Checking Report identifies plants that are missing from a State's data submission or that reported substantially different emissions from previous years. Facilities emitting over 1000 tons in 1985 are compared to 1000 ton emitters for 1984. Large discrepancies are tabulated. Plants in the 1984 listing, but not in the 1985 listing, are also tabulated. Another list, the Independent Completeness File, is compiled of plants in industries that contribute a significant percentage to nationwide point source emissions. References for this list include trade association publications,[5,6,7,8,9] current industrial directories,[10,11,12,13,14] EPA New Source Performance Standards files,[15,16,17,18,19,20,21,22] and EPA's Best Available Control Technology (BACT)/Lowest Achievable Emission Rate (LAER) Clearinghouse. Plants in the Independent Completeness File, but not in the 1985 NEDS list, are also flagged.

The Parameter Range Validation Report contains output from the final computerized check. The report compares data items to a statistical range for the data item based on the process or SCC code. A valid range for the data item was arbitrarily set at 2.5 standard deviations outside the mean for a given SCC. Parameters of interest in this report include stack parameters, control device efficiency, fuel parameters, and operating rate data. Data items included in this report do not necessarily contain errors. This report identifies data items that fall signficantly outside the limits of what is normally encountered for that parameter in the SCC group. The data items are reviewed, and the items that are deemed truly questionable are flagged manually. Flagged items are brought to the attention of the submitting agency for confirmation or correction and resubmission.

The last section of the QA/QC report, titled Miscellaneous QA Questions, lists problems encountered during the second screening of the data (described above), including over-reported fuel consumption, miscoded SCCs, and instances where NEDS encountered problems with computer-calculated emissions.

The six QA/QC sections are assembled into one document, which is returned to the State and EPA regional offices for review, comment, and corrective action. This review process ensures that the data comprising the 1985 emissions inventory will be endorsed by both States and EPA. As the data are corrected and as default values are substituted for missing data, a computerized audit tracking system keeps track of all changes to the original State-submitted data. In addition, State confirmation of suspect values is tracked. The audit trail tracks changes made to the data and ensures that all identified problems have been addressed.

Utility Quality Control Checks

Utilities represent the single largest point source category of NO_x and SO_x emissions. For this reason, a comprehensive methodology of QA/QC checks was developed specifically for this source category. The focus of this methodology is on complete coverage of the electric utility industry, proper classification of all electric utilities, and agreement between specific data reported to EPA and data reported to DOE.

The first part of this methodology is a review of NEDS data to identify plants that may be electric utilities. The first three digits of the SCC codes for electric utility boilers are 101 or 102. In addition, the Standard Industrial Classification (SIC) code for electric utilities is 4911. The review identifies both facilities meeting these criteria and facilities which partially meet the criteria but appear to have internally inconsistent data. The utilities found in NEDS are compared to those provided by DOE. In order to ensure that all potentially large utilities are covered, all discrepancies that involve utilities expected to emit at least 100 TPY of NO_x, SO_x, or VOC are noted.

The second part of the electric utility review is a direct comparison of data elements reported by the utility plants to EPA through NEDS and to DOE through Energy Information Administration (EIA) Form 767. The NAPAP high priority data elements are of particular concern. This report is assembled and distributed to the States, once again allowing them to comment on the validity of the suspect data encountered during this QA/QC process.

QUALITY CONTROL OF THE NAPAP INVENTORY

Area sources are defined to include all mobile sources of emissions and stationary sources whose individual emissions are too small to be included in the NAPAP point source inventory. The area source data are needed by NAPAP to provide a full accounting of emissions from all sources during 1985. The U.S. EPA's Office of Air Quality Planning and Standards (OAQPS) develops the area source emission files. Once they have been developed they are sent to the State and Regional Offices for comment and review. The NEDS point and area source emissions files constitute the raw data of the NAPAP inventory. A computer program [termed the Flexible Regional Emission Data System (FREDS)] extracts the necessary data from NEDS and applies appropriate temporal, spatial, and pollutant species allocation factors to derive a gridded, speciated, and temporally resolved emissions file suitable for input to regional scale atmospheric models. A flow chart of FREDS is presented in Figure 2.

A two step process ensures the quality of the completed NAPAP inventory. First, the allocation factors are examined for reasonableness. Second, after the factors are applied to the raw data, the resulting inventory is examined for spurious results. Due to the size and complexity of the completed inventory, special techniques were developed for QA/QC of the inventory. This section will focus on this second step, the QA/QC measures applied to the completed inventory.

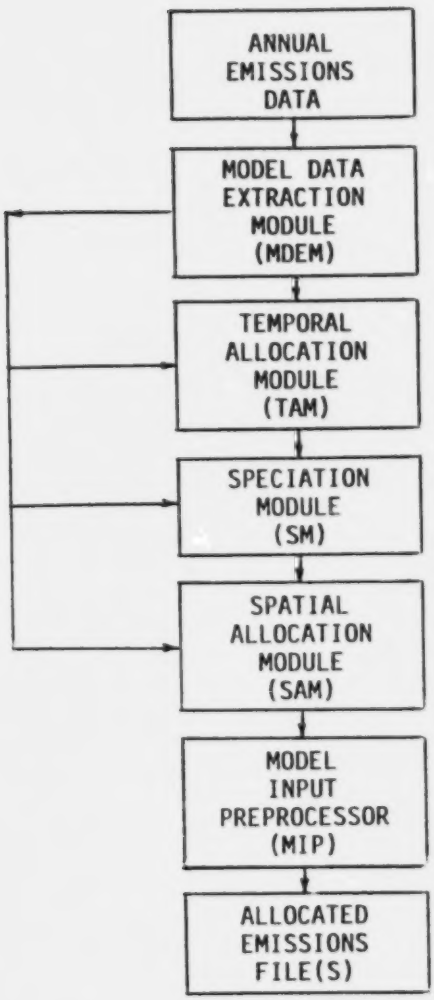

Figure 2. Flow Chart of the Flexible Regional Emissions Data System (FREDS)

Three types of allocation factors are used in the FREDS program: spatial, temporal, and species. These factors were developed for area and point source categories used in the Northeast Corridor Regional Modeling Project (NECRMP).[23] Additional factors were developed for the additional source categories and areas included in NAPAP.

The area source county emissions are allocated to grid cells based on surrogate data such as population, housing, or employment statistics. A direct visual comparison of the allocated emission estimates to surrogates used to develop the estimates can quickly isolate potential problems by illustrating different patterns in the data. For example, VOC emissions from degreasing and dry cleaning are allocated to grid cells using population data. Plots of VOC emissions from these industries should have patterns that match the plot of population data.

The allocated emission estimates are summed at the county, State, and National levels. These totals are compared to the original emissions data in NEDS to ensure that there are no errors in the spatial allocation factors.

A common problem of past inventories involved the discontinuity of emission estimates at geopolitical borders. After the emissions are plotted, the grid cell, county, and State boundaries are overlayed to determine if these types of errors exist. A sample plot is presented in Figure 3. These errors can indicate errors in the allocation factors, differences in methodologies used by different State or sub-State emission estimators, or in the application or selection of the allocation factors.

Data from land use maps are used in the development of spatial allocation factors for such categories as VOC emissions from forest fires. The allocated emissions are plotted as a function of concentration for large categories and compared to the original land use maps to identify differences in the data patterns.

The annual totals for the major pollutant species (NO_x, SO_x, and VOC) are plotted. For this analysis, TSP is also plotted. Physical boundaries such as mountain ranges, rivers, and lakes should be easily distinguished by their lack of emissions.

Hourly operating data are plotted as a function of time for major source categories. These plots are analyzed to ensure that the zero and 24 hour data are in agreement. In addition the curves are checked for reasonableness. Patterns should match 8 or 16 hour manufacturing shifts. Utility data should illustrate peak load times.

The speciation of the data is checked by summing the speciated data and checking it against the original data. For example the total nitrogen oxide (NO) and nitrogen dioxide (NO_2) emission levels should equal the original NO_x estimates.

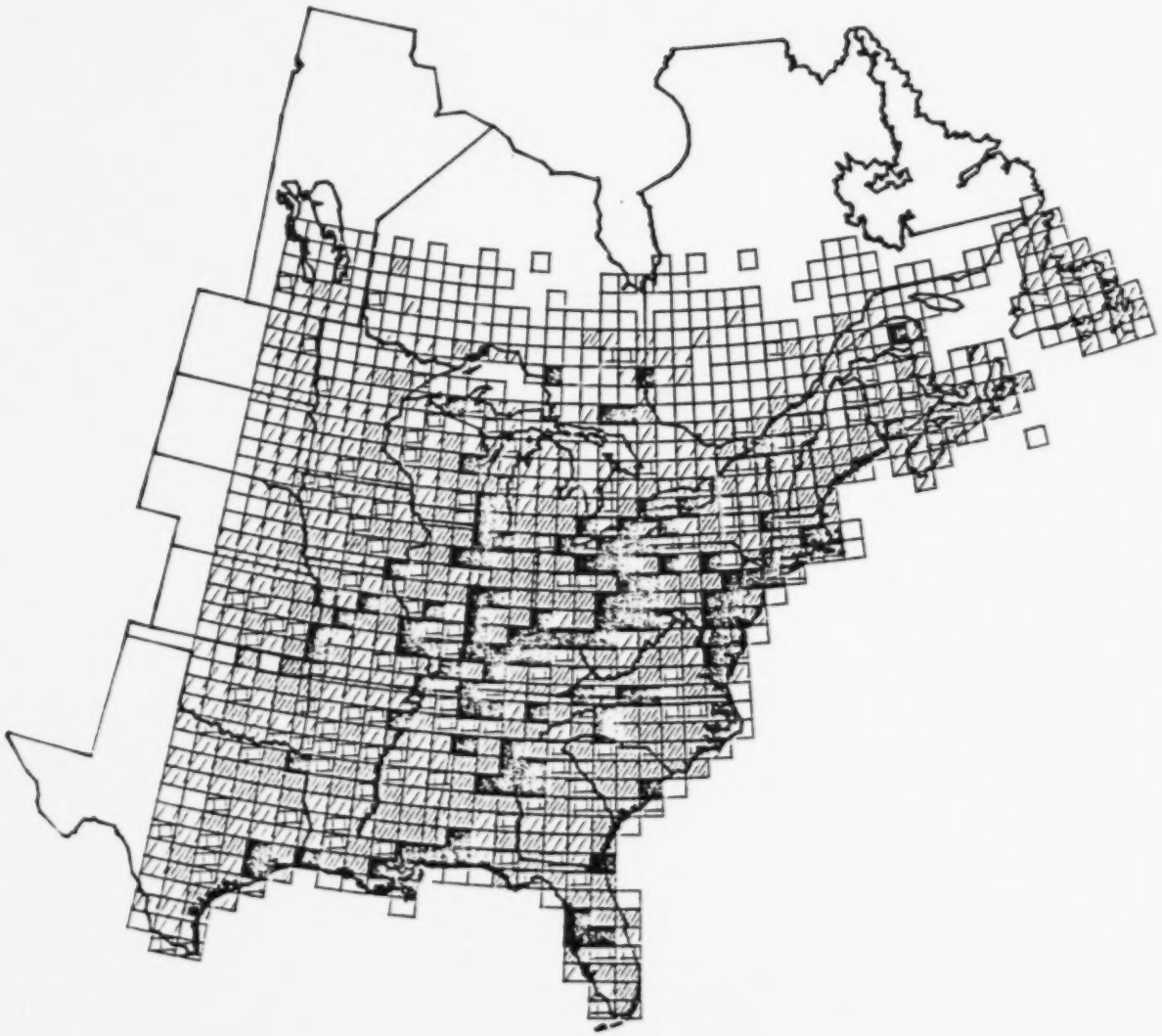

Figure 3. Daily SO_2 Emissions for a Summer Weekday
(1980 NAPAP Inventory)

CONCLUSION

The extensive QA/QC procedures outlined in this paper are being applied to ensure an accurate, reliable, and validated data base. The 1985 NAPAP Emissions Inventory is scheduled for release to the user community in January of 1988.[24] The quality of this data base will go far in providing the best answers to the questions of how anthropogenic emissions contribute to and affect acid rain precursors.

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